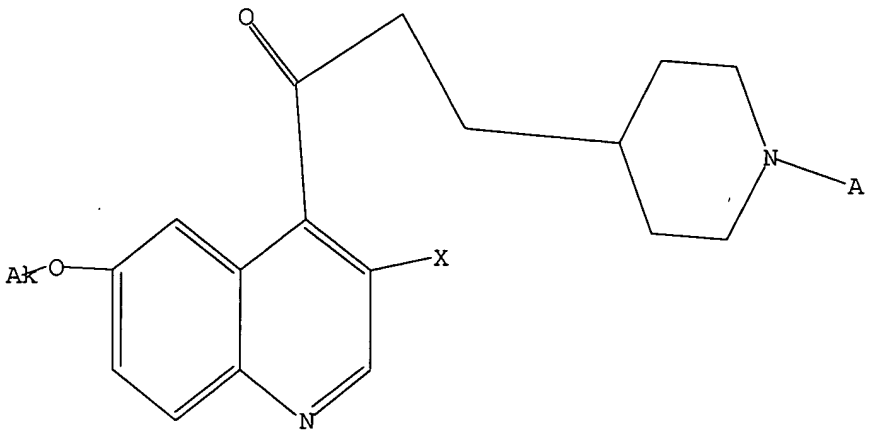
L5 STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5 STR



G1 Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l5 full
FULL SEARCH INITIATED 21:33:56 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 600 TO ITERATE

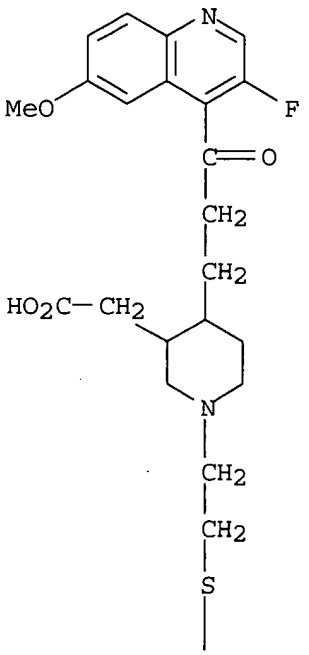
100.0% PROCESSED 600 ITERATIONS 15 ANSWERS
SEARCH TIME: 00.00.01

L6 15 SEA SSS FUL L5

=> d l6 1-15

L6 ANSWER 1 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-39-6 REGISTRY
ED Entered STN: 29 Mar 2004
CN 3-Piperidineacetic acid, 1-[2-[(2,5-difluorophenyl)thio]ethyl]-4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)
MF C28 H29 F3 N2 O4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A



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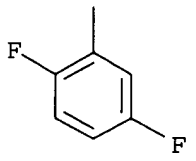
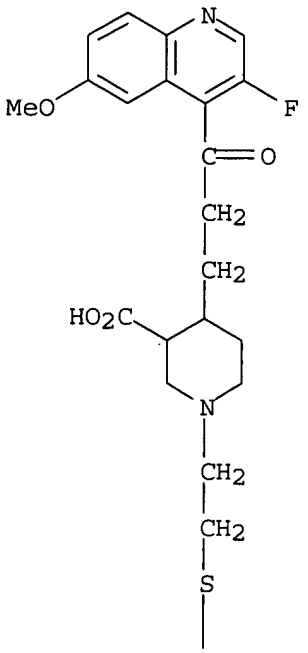


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 2 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-38-5 REGISTRY
ED Entered STN: 29 Mar 2004
CN 3-Piperidinecarboxylic acid, 1-[2-[(2,5-difluorophenyl)thio]ethyl]-4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 4-[3-Oxo-3-(3-fluoro-6-methoxyquinolin-4-yl)propyl]-1-[2-[(2,5-difluorophenyl)sulfanyl]ethyl]piperidine-3-carboxylic acid
MF C27 H27 F3 N2 O4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A



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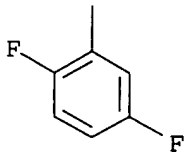
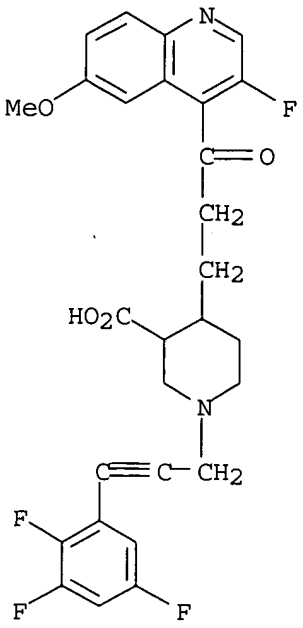


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 3 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-37-4 REGISTRY
ED Entered STN: 29 Mar 2004
CN 3-Piperidinecarboxylic acid, 4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-1-[3-(2,3,5-trifluorophenyl)-2-propynyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 4-[3-(3-Fluoro-6-methoxyquinolin-4-yl)-3-oxopropyl]-1-[3-(2,3,5-trifluorophenyl)prop-2-ynyl]piperidine-3-carboxylic acid
MF C28 H24 F4 N2 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

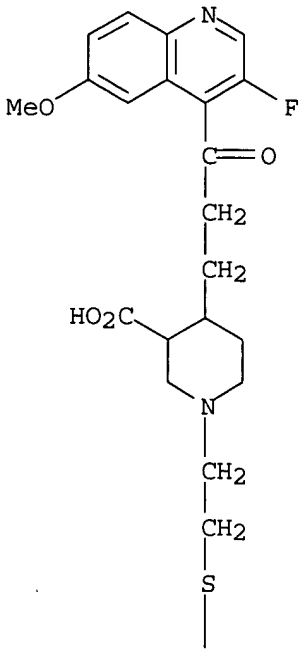


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 4 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-36-3 REGISTRY
ED Entered STN: 29 Mar 2004
CN 3-Piperidinecarboxylic acid, 1-[2-(cyclohexylthio)ethyl]-4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-[2-(Cyclohexylsulfanyl)ethyl]-4-[3-(3-fluoro-6-methoxyquinolin-4-yl)-3-oxopropyl]piperidine-3-carboxylic acid
MF C27 H35 F N2 O4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A



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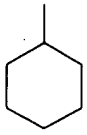
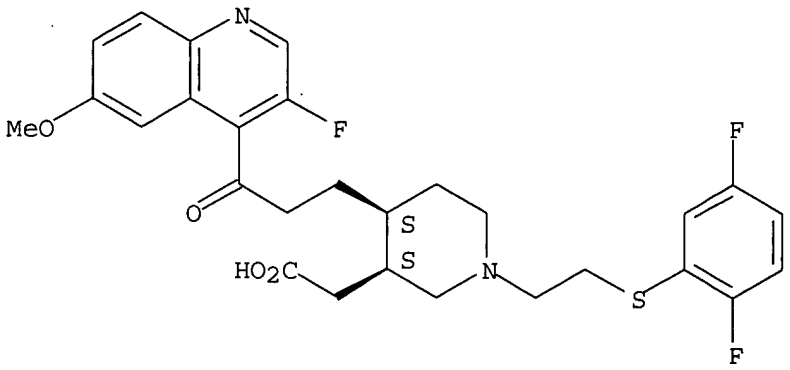


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 5 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-30-7 REGISTRY
ED Entered STN: 29 Mar 2004
CN 3-Piperidineacetic acid, 1-[2-[(2,5-difluorophenyl)thio]ethyl]-4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-, (3R,4R)-rel- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (3RS,4RS)-4-[3-Oxo-3-(3-fluoro-6-methoxyquinolin-4-yl)propyl]-1-[2-[(2,5-difluorophenyl)sulfanyl]ethyl]piperidine-3-acetic acid
FS STEREOSEARCH
MF C28 H29 F3 N2 O4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Relative stereochemistry.

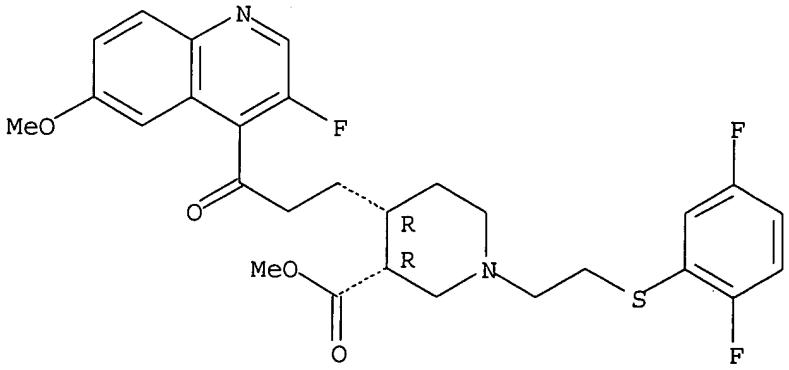


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 6 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-29-4 REGISTRY
ED Entered STN: 29 Mar 2004
CN 3-Piperidinecarboxylic acid, 1-[2-[(2,5-difluorophenyl)thio]ethyl]-4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-, methyl ester, (3R,4R)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Methyl (3R,4R)-4-[3-oxo-3-(3-fluoro-6-methoxyquinolin-4-yl)propyl]-1-[2-[(2,5-difluorophenyl)sulfanyl]ethyl]piperidine-3-carboxylate
FS STEREOSEARCH
MF C28 H29 F3 N2 O4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



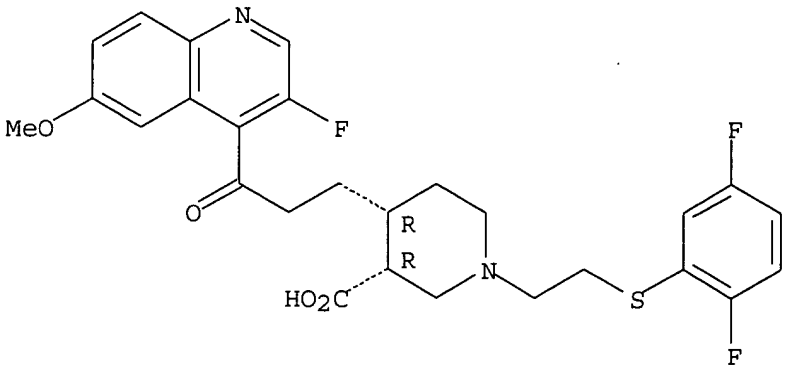
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 7 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-28-3 REGISTRY
ED Entered STN: 29 Mar 2004

CN 3-Piperidinecarboxylic acid, 1-[2-[(2,5-difluorophenyl)thio]ethyl]-4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-, (3R,4R)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (3R,4R)-4-[3-Oxo-3-(3-fluoro-6-methoxyquinolin-4-yl)propyl]-1-[2-[(2,5-difluorophenyl)sulfanyl]ethyl]piperidine-3-carboxylic acid
FS STEREOSEARCH
MF C27 H27 F3 N2 O4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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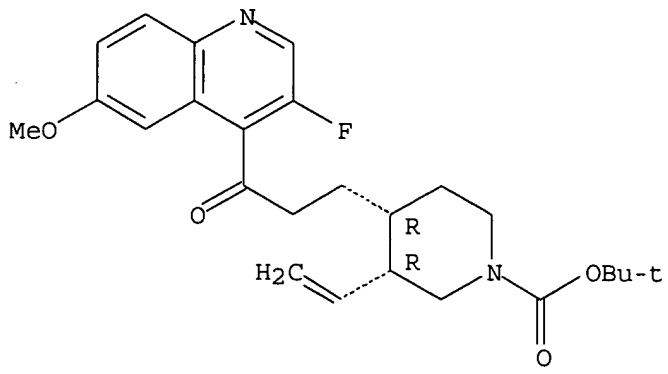
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 8 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-25-0 REGISTRY
ED Entered STN: 29 Mar 2004
CN 1-Piperidinecarboxylic acid, 3-ethenyl-4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-, 1,1-dimethylethyl ester, (3R,4R)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (3R,4R)-1-(tert-Butyloxycarbonyl)-4-[3-(3-fluoro-6-methoxyquinolin-4-yl)-3-oxopropyl]-3-vinylpiperidine
FS STEREOSEARCH
MF C25 H31 F N2 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

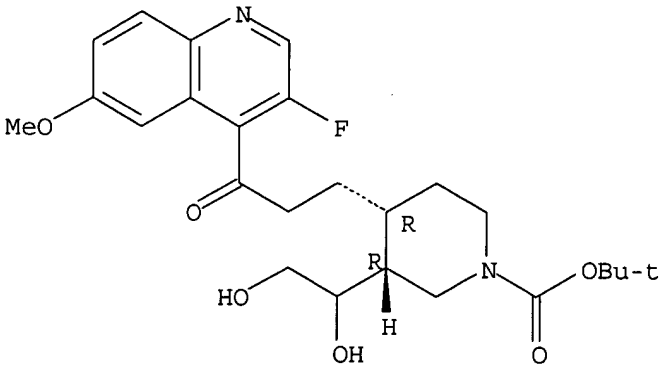


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 9 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-24-9 REGISTRY
ED Entered STN: 29 Mar 2004
CN 1-Piperidinecarboxylic acid, 3-(1,2-dihydroxyethyl)-4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-, 1,1-dimethylethyl ester, (3R,4R)-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H33 F N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



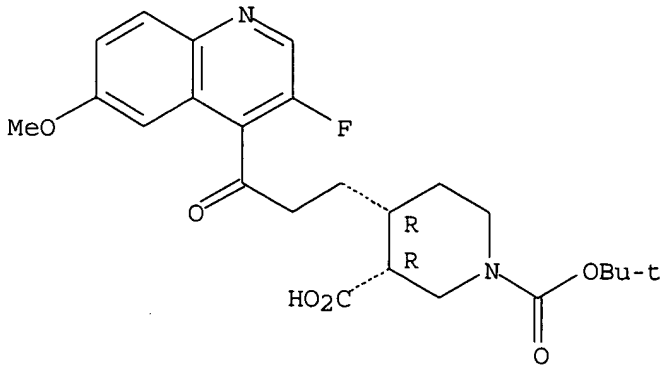
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 10 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-23-8 REGISTRY
ED Entered STN: 29 Mar 2004
CN 1,3-Piperidinedicarboxylic acid, 4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-, 1-(1,1-dimethylethyl) ester, (3R,4R)- (9CI) (CA INDEX NAME)
OTHER NAMES:

CN (3R,4R)-1-(tert-Butyloxycarbonyl)-4-[3-(3-fluoro-6-methoxyquinolin-4-yl)-3-oxopropyl]piperidine-3-carboxylic acid
FS STEREOSEARCH
MF C24 H29 F N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

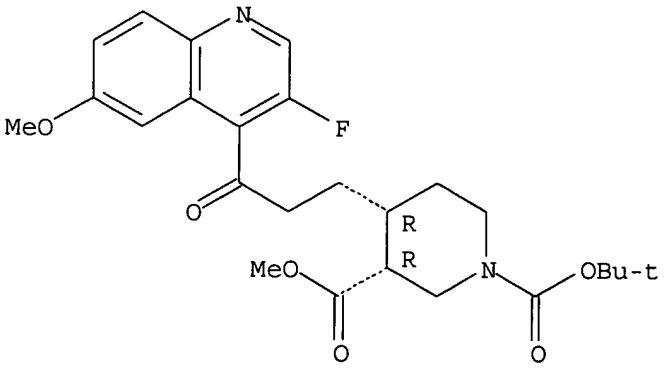


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 11 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-22-7 REGISTRY
ED Entered STN: 29 Mar 2004
CN 1,3-Piperidinedicarboxylic acid, 4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-, 1-(1,1-dimethylethyl) 3-methyl ester, (3R,4R)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Methyl (3R,4R)-1-(tert-butyloxycarbonyl)-4-[3-(3-fluoro-6-methoxyquinolin-4-yl)-3-oxopropyl]piperidine-3-carboxylate
FS STEREOSEARCH
MF C25 H31 F N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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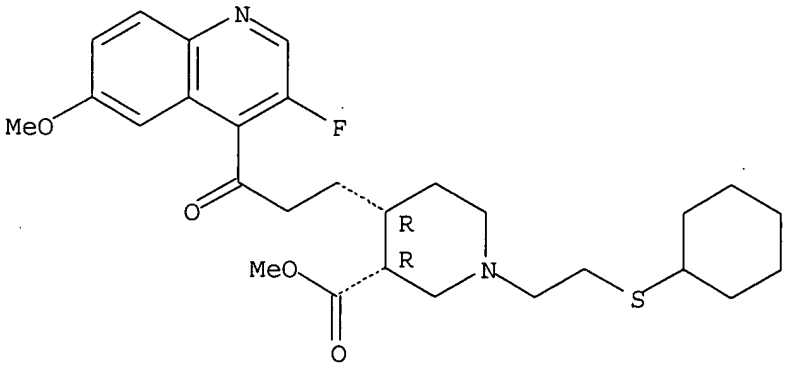
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 12 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-20-5 REGISTRY
ED Entered STN: 29 Mar 2004
CN 3-Piperidinecarboxylic acid, 1-[2-(cyclohexylthio)ethyl]-4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-, methyl ester, (3R,4R)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Methyl (3R,4R)-1-[2-(cyclohexylsulfanyl)ethyl]-4-[3-(3-fluoro-6-methoxyquinolin-4-yl)-3-oxopropyl]piperidine-3-carboxylate
FS STEREOSEARCH
MF C28 H37 F N2 O4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

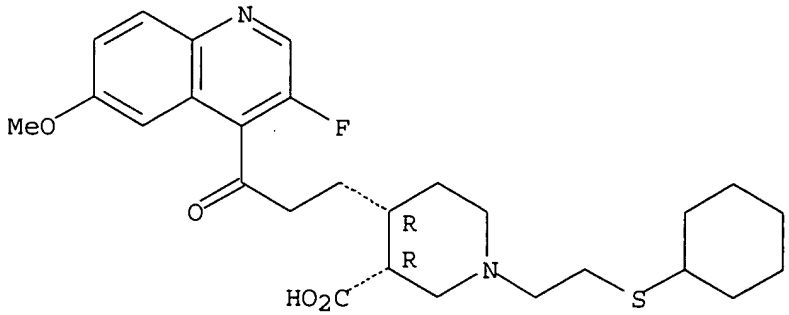


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 13 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 668463-19-2 REGISTRY
ED Entered STN: 29 Mar 2004
CN 3-Piperidinecarboxylic acid, 1-[2-(cyclohexylthio)ethyl]-4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-, (3R,4R)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (3R,4R)-1-[2-(Cyclohexylsulfanyl)ethyl]-4-[3-(3-fluoro-6-methoxyquinolin-4-yl)-3-oxopropyl]piperidine-3-carboxylic acid
FS STEREOSEARCH
MF C27 H35 F N2 O4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

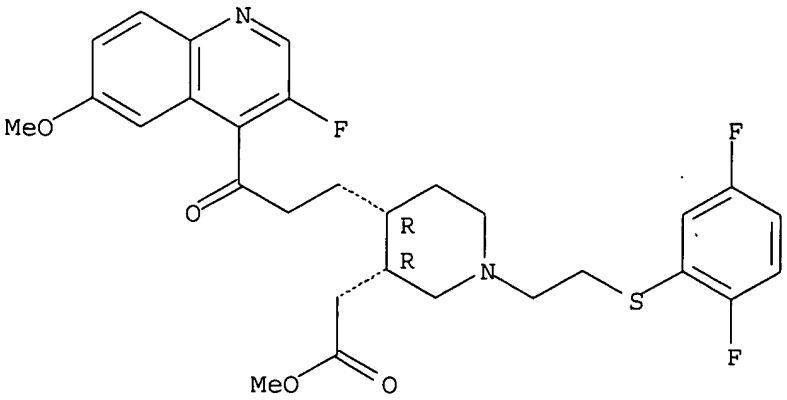


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 14 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 459453-11-3 REGISTRY
ED Entered STN: 07 Oct 2002
CN 3-Piperidineacetic acid, 1-[2-[(2,5-difluorophenyl)thio]ethyl]-4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-, methyl ester, (3R,4R)-rel- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (3RS,4RS)-Methyl 4-[3-oxo-3-(3-fluoro-6-methoxyquinolin-4-yl)propyl]-1-[2-[(2,5-difluorophenyl)thio]ethyl]piperidine-3-acetate
CN Methyl (3RS,4RS)-4-[3-oxo-3-(3-fluoro-6-methoxyquinolin-4-yl)propyl]-1-[2-[(2,5-difluorophenyl)sulfanyl]ethyl]piperidine-3-acetate
FS STEREOSEARCH
MF C29 H31 F3 N2 O4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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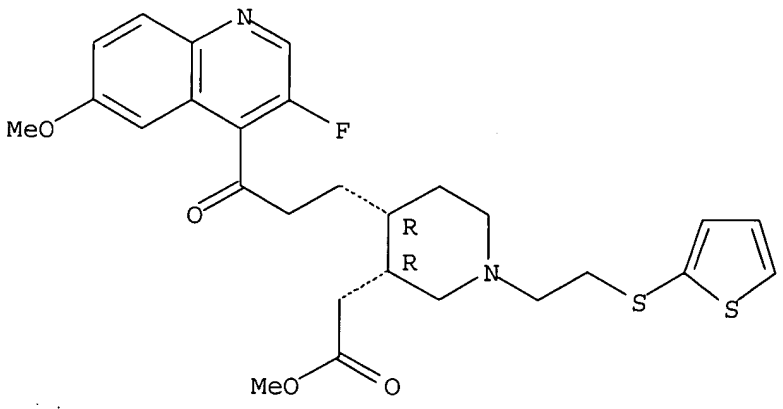
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 15 OF 15 REGISTRY COPYRIGHT 2006 ACS on STN
RN 459453-07-7 REGISTRY
ED Entered STN: 07 Oct 2002
CN 3-Piperidineacetic acid, 4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-1-[2-(2-thienylthio)ethyl]-, methyl ester, (3R,4R)-rel- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (3RS,4RS)-Methyl 4-[3-oxo-3-(3-fluoro-6-methoxyquinolin-4-yl)propyl]-1-[2-(2-thienylthio)ethyl]piperidine-3-acetate
FS STEREOSEARCH
MF C27 H31 F N2 O4 S2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:716269 CAPLUS
DOCUMENT NUMBER: 137:232568
TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials
INVENTOR(S): Bacque, Eric; Mignani, Serge; Malleron, Jean-Luc; Tabart, Michel; Evers, Michel; Viviani, Fabrice; El-Ahmad, Youssef; Mutti, Stephane; Daubie, Christophe
PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
SOURCE: PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072572	A1	20020919	WO 2002-FR851	20020311
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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FR 2822154	B1	20051021		
CA 2440067	AA	20020919	CA 2002-2440067	20020311
EP 1370550	A1	20031217	EP 2002-722329	20020311
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US 2002177606	A1	20021128	US 2002-96482	20020313
US 6602884	B2	20030805		
US 2003171369	A1	20030911	US 2003-387479	20030314
US 6815547	B2	20041109		

PRIORITY APPLN. INFO.:

FR 2001-3374	A	20010313
US 2001-281407P	P	20010405
WO 2002-FR851	W	20020311
US 2002-96482	A3	20020313

OTHER SOURCE(S): MARPAT 137:232568
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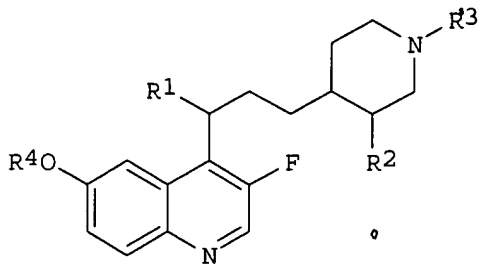

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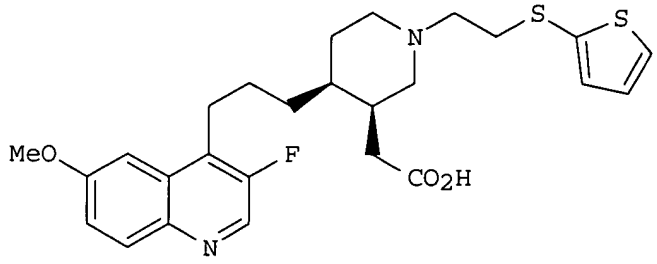


II

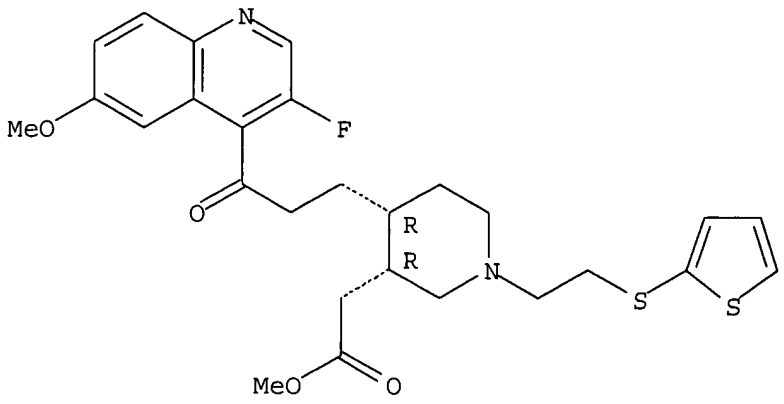
AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1 = H, halo, OH, NH2, alkylamino, dialkylamino, hydroxyamino, alkoxyamino, or alkylalkoxyamino; R2 = COOH, CH2CO2H, CH2OH; R3 = C1-6 alkyl substituted by: (un)substituted SPh [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered aromatic heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl containing 3 -7 members, or by 5- to 6-membered aromatic heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = C1-6 alkyl, alkenyl-CH2, or alkynyl-CH2- (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including diastereoisomeric forms, mixts. thereof, cis or trans forms, and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Ten synthetic examples are given. For instance, Wittig reaction of 4(RS)-4-allyl-1-(benzyloxycarbonyl)piperidin-3-one with Ph3P:CHCO2Me gave a Z-isomeric exocyclic olefin, which underwent hydroboration at allyl and Pd-catalyzed coupling with 4-iodo-3-fluoro-6-methoxyquinoline, followed by hydrogenation of the olefin with concomitant N-deprotection, N-alkylation with 2-(2-bromoethylthio)thiophene, and saponification of the Me ester, to give the racemic title compound II.2HCl. Compds. I were active against exptl. infections of mice by Staphylococcus aureus IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).

IT 459453-07-7P, (3RS,4RS)-Methyl 4-[3-oxo-3-(3-fluoro-6-methoxyquinolin-4-yl)propyl]-1-[2-[(2-thienyl)thio]ethyl]piperidine-3-acetate 459453-11-3P, (3RS,4RS)-Methyl 4-[3-oxo-3-(3-fluoro-6-methoxyquinolin-4-yl)propyl]-1-[2-[(2,5-difluorophenyl)thio]ethyl]piperidine-3-acetate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (quinolylpropyl)piperidine derivs. as antimicrobials)

RN 459453-07-7 CAPLUS

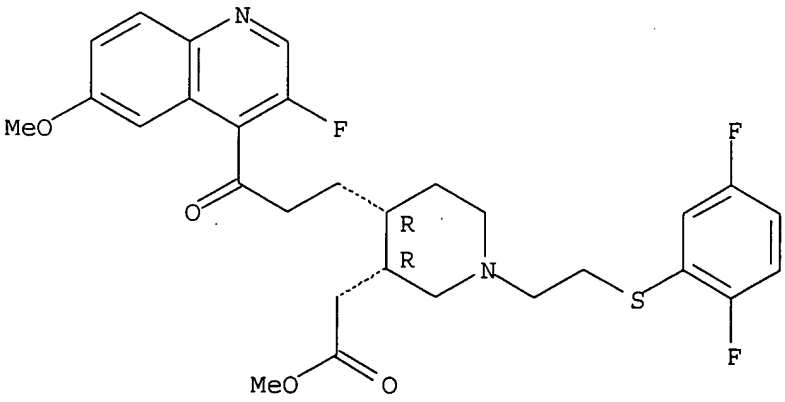
CN 3-Piperidineacetic acid, 4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-1-[2-(2-thienylthio)ethyl]-, methyl ester, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 459453-11-3 CAPLUS
CN 3-Piperidineacetic acid, 1-[2-[(2,5-difluorophenyl)thio]ethyl]-4-[3-(3-fluoro-6-methoxy-4-quinolinyl)-3-oxopropyl]-, methyl ester, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:80192 CAPLUS
DOCUMENT NUMBER: 140:146015
TITLE: Preparation of quinolylpropylpiperidines as antimicrobial agents
INVENTOR(S): Bacque, Eric; Malleron, Jean Luc; Mignani, Serge; Tabart, Michel
PATENT ASSIGNEE(S): Aventis Pharma SA, Fr.
SOURCE: Fr. Demande, 39 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2842807	A1	20040130	FR 2002-9334	20020723
US 2004058919	A1	20040325	US 2003-622655	20030718
US 6806277	B2	20041019		
WO 2004011454	A2	20040205	WO 2003-FR2306	20030722
WO 2004011454	A3	20040408		
W: AE, AG, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CO, CR, CU, CZ, DM, DZ, EC, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, OM, PH, PL, RO, SC, SG, SK, TN, TT, UA, UZ, VC, VN, YU, ZA				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003267528	A1	20040216	AU 2003-267528	20030722
PRIORITY APPLN. INFO.:			FR 2002-9334 A	20020723
			WO 2003-FR2306 W	20030722

OTHER SOURCE(S): MARPAT 140:146015
GI

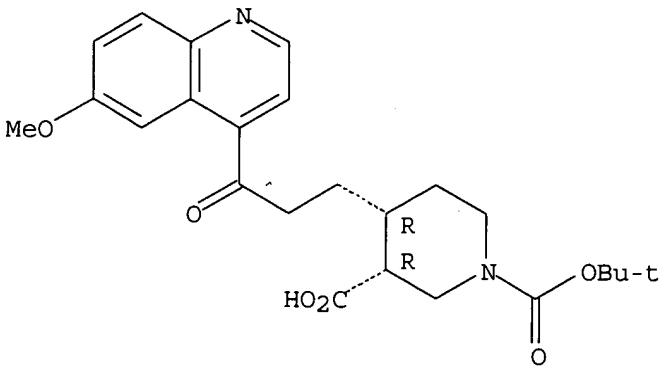
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [wherein R1 = alkyl/dialkyl/hydroxy/alkyloxy/ alkyl alkyloxy/amino; R2 = carboxy, carboxymethyl, hydroxymethyl; R3 = (un)substituted alkyl, propargyl; R4 = alkyl, alkenyl-CH2 -, alkynyl-CH2-, cycloalkyl, cycloalkylalkyl; diastereoisomeric forms, mixts. thereof, cis or trans forms, and their salts] were prepared as antimicrobial agents. Two synthetic examples are given. For example, II was prepd in 7 steps from olefin III by oxidation with NaMnO4 to the acid concomitant with N-BOC-protection, esterification, followed by BOC deprotection, N-alkylation with propargylic alc., reaction of the resulting alkyne with 1-bromo-2,3,5-trifluorobenzene, oximation, reduction of the oxime, and hydrolysis of the ester. I were active against exptl. infections of mice by Staphylococcus aureus IP8203 at 65 mg/kg s.c., and at 70 mg/kg orally. None of the compds. showed acute toxicity in mice at 100 mg/kg s.c. (2 administrations).

IT 333782-31-3P, (3R,4R)-4-[3-Oxo-3-(6-methoxyquinolin-4-yl)propyl]-1-(tert-butyloxycarbonyl)piperidine-3-carboxylic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of quinolylpropylpiperidines as antimicrobial agents)

RN 333782-31-3 CAPLUS
CN 1,3-Piperidinedicarboxylic acid, 4-[3-(6-methoxy-4-quinolinyl)-3-oxopropyl]-, 1-(1,1-dimethylethyl) ester, (3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:265410 CAPLUS
DOCUMENT NUMBER: 134:280720
TITLE: Quinolylpropylpiperidines with antibacterial activity
INVENTOR(S): Malleron, Jean-Luc; Tabart, Michel; Carry, Jean-Christophe; Evers, Michel; El Ahmad, Youssef; Mignani, Serge; Viviani, Fabrice
PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
SOURCE: PCT Int. Appl., 305 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

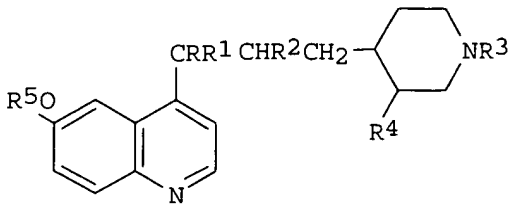
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001025227	A2	20010412	WO 2000-FR2541	20000914
WO 2001025227	A3	20011122		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2798656	A1	20010323	FR 1999-11679	19990917
FR 2798656	B1	20041217		
CA 2383836	AA	20010412	CA 2000-2383836	20000914
BR 2000014060	A	20020521	BR 2000-14060	20000914
EP 1218370	A2	20020703	EP 2000-962637	20000914
EP 1218370	B1	20041208		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
EE 200200138	A	20030616	EE 2002-138	20000914
JP 2004527448	T2	20040909	JP 2001-528171	20000914
EP 1484328	A1	20041208	EP 2004-19136	20000914

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, LT, LV, FI, MK, CY

AT 284399	E	20041215	AT 2000-962637		20000914
US 6403610	B1	20020611	US 2000-664959		20000918
NO 2002001253	A	20020424	NO 2002-1253		20020313
ZA 2002002073	A	20030613	ZA 2002-2073		20020313
BG 106524	A	20030131	BG 2002-106524		20020315
PRIORITY APPLN. INFO.:			FR 1999-11679	A	19990917
			US 1999-162225P	P	19991029
			EP 2000-962637	A3	20000914
			WO 2000-FR2541	W	20000914

OTHER SOURCE(S): MARPAT 134:280720

GI



I

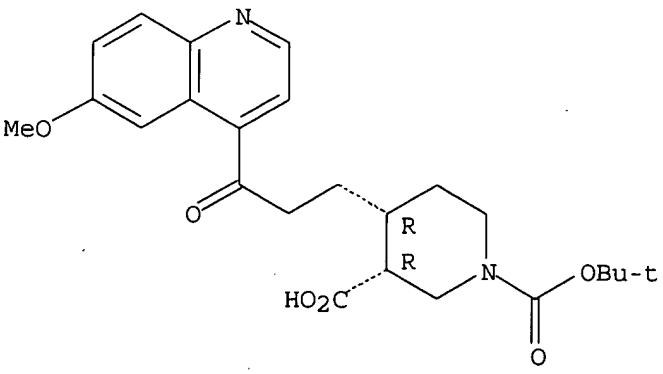
AB Title compds. I [R = H, halogen, OH; R1 = H or halogen when R = halogen; R2 = H; R1R2 = bond, R = H; R3 = (un)substituted alkyl, propargyl, cinnamyl, 4-phenyl-3-butenyl; R4 = (un)esterified CO2H, CH2CO2H, CH2CH2CO2H, CH2OH; R5 = alkyl, alkenyl, alkynyl] were prepared for use as antibacterial agents (no data). Thus, (3R,4R)-4-[3-(6-methoxyquinolin-4-yl)propyl]-1-(3-phenylpropyl)piperidine-3-carboxylic acid was prepared from (3R,4R)-4-[3-(6-methoxyquinolin-4-yl)propyl]-3-vinylpiperidine by benzoylation, reaction with 1-bromo-3-phenylpropane, and ester hydrolysis.

IT 333782-31-3P 333783-09-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinolylpropylpiperidines with antibacterial activity)

RN 333782-31-3 CAPLUS

CN 1,3-Piperidinedicarboxylic acid, 4-[3-(6-methoxy-4-quinolinyl)-3-oxopropyl]-, 1-(1,1-dimethylethyl) ester, (3R,4R)- (9CI) (CA INDEX NAME)

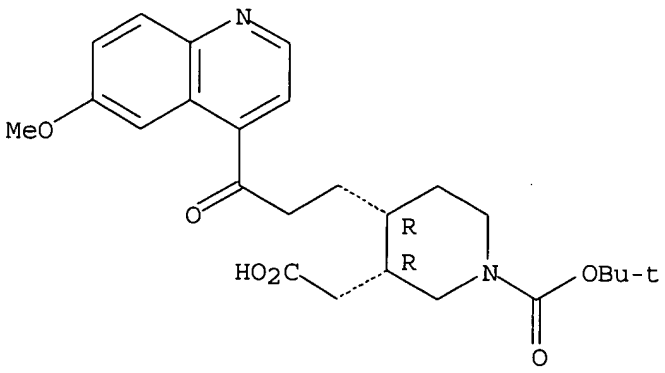
Absolute stereochemistry.



RN 333783-09-8 CAPLUS

CN 3-Piperidineacetic acid, 1-[(1,1-dimethylethoxy)carbonyl]-4-[3-(6-methoxy-4-quinolinyl)-3-oxopropyl]-, (3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

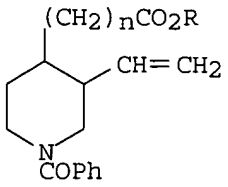

N
MeO
O
R
R
HO2C
N
OBu-t
O

=>

L3 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:577748 CAPLUS
DOCUMENT NUMBER: 85:177748
TITLE: Processes and intermediates for cis or trans 2- or 3-(1-acyl-3-vinyl-4-piperidine)acetic or propionic acid esters
INVENTOR(S): Grethe, Guenter; Uskokovic, Milan R.
PATENT ASSIGNEE(S): Hoffmann-La Roche, Inc., USA
SOURCE: U.S., 15 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3959294	A	19760525	US 1975-580493	19750523
PRIORITY APPLN. INFO.:			US 1970-100370 A3	19701221
			US 1973-362604 A3	19730521

GI



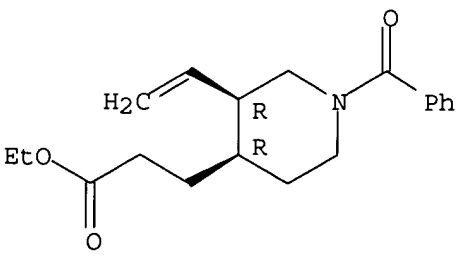
I

AB The title compds. (±)-cis- and (±)-trans-, 3,4-(S)-, 3,4-(R)-I; (n = 1,2; R = H, Me, Et) were prepared Thus, Et cis-(3-ethyl-4-piperidinepropionate was chlorinated with N-chlorosuccinimide and the N-chloro deriv irradiated in F3CCO2H to give Et cis-3-(2-chloroethyl)-4-piperidinepropionate-F3CCO2H, which was treated with PhCOCl followed with NaI and dehydriodination to give (±)-cis-I (n = 2, R = Et).

IT 26847-64-3P 26847-65-4P 60384-93-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

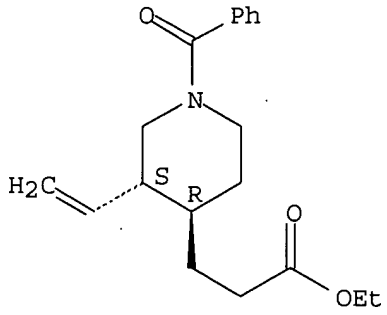
RN 26847-64-3 CAPLUS
CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



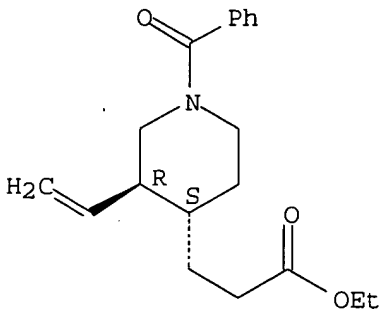
RN 26847-65-4 CAPLUS
CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, (3S-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 60384-93-2 CAPLUS
CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, (3R-trans)-(9CI) (CA INDEX NAME)

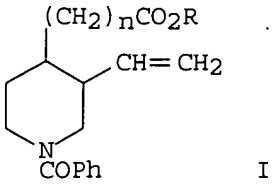
Absolute stereochemistry.



L3 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:577747 CAPLUS
DOCUMENT NUMBER: 85:177747
TITLE: Processes and intermediates for cis or trans 2- or 3-(1-acyl-3-vinyl-4-piperidine)acetic or propionic acid esters
INVENTOR(S): Grethe, Guenter; Uskokovic, Milan R.
PATENT ASSIGNEE(S): Hoffmann-La Roche, Inc., USA
SOURCE: U.S., 15 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3957800	A	19760518	US 1975-580492	19750523
PRIORITY APPLN. INFO.:			US 1970-100370 A3	19701221
			US 1973-362604 A3	19730521

GI



I

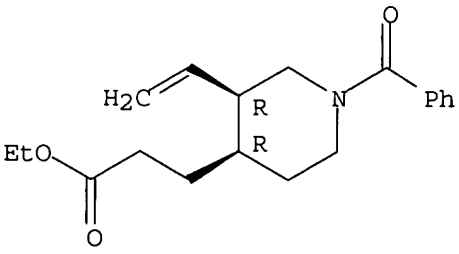
AB The title compds. (±)-cis- and (±)-trans-, 3,4-(S)-, 3,4-(R)-I; (n = 1,2; R = H, Me, Et) were prepared Thus, Et cis-3-ethyl-4-piperidinepropionate was chlorinated with N-chlorosuccinimide and, the N-chloro derivative irradiated in F3CCO2H to give Et cis-3-(2-chloroethyl)-4-piperidinepropionate-F3CCO2H, which was treated with PhCOCl followed treatment with NaI and dehydriodination to give (±)-cis-I (n = 2, R = Et).

IT 26847-64-3P 26847-65-4P 60384-93-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 26847-64-3 CAPLUS

CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, cis- (9CI) (CA INDEX NAME)

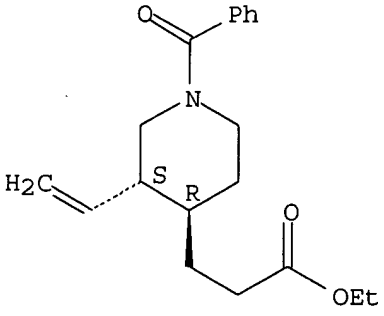
Relative stereochemistry.



RN 26847-65-4 CAPLUS

CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, (3S-trans)-(9CI) (CA INDEX NAME)

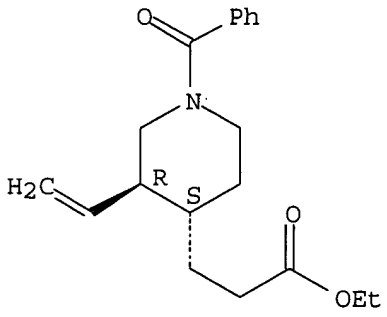
Absolute stereochemistry.



RN 60384-93-2 CAPLUS

CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, (3R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

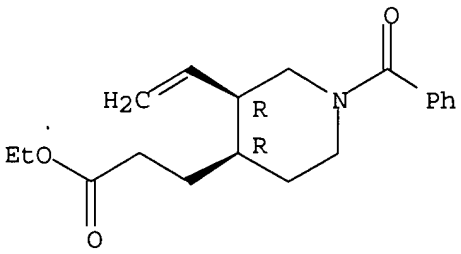


L3 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1974:552024 CAPLUS
DOCUMENT NUMBER: 81:152024
TITLE: 3-(2-Chloroethyl)-4-piperidineacetic acid and esters
INVENTOR(S): Grethe, Guenter; Radoje, Milan
PATENT ASSIGNEE(S): Hoffmann-La Roche, Inc.
SOURCE: U.S., 11 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3833593	A	19740903	US 1973-367307	19730605
PRIORITY APPLN. INFO.:			US 1970-100370 A2	19701221

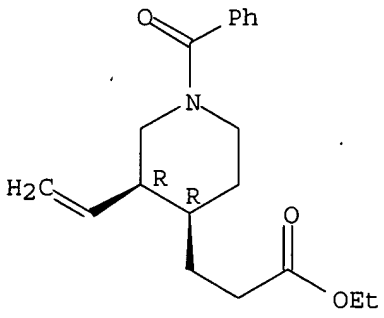
GI For diagram(s), see printed CA Issue.
AB Piperidinealkanoates I (n = 1, R = Me; n = 2, R = Et) were prepared as intermediates for antimalarial and antiarrhythmic quinine and quinidine derivs. Thus, II (R1 = Et, R2 = H) was N-chlorinated, photochem. rearranged to II (R1 = CH2CH2Cl, R2 = H), benzoylated, iodinated to II (R1 = CH2CH2I, R2 = Bz), and dehydrohalogenated to give II (R1 = vinyl, R2 = Bz).
IT 26847-64-3P 26847-66-5P 42881-64-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 26847-64-3 CAPLUS
CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



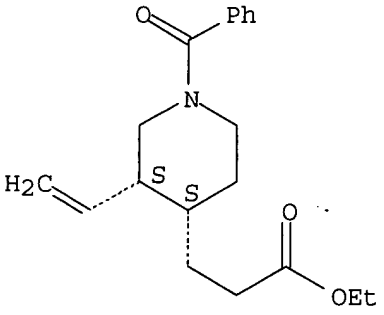
RN 26847-66-5 CAPLUS
CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, (3R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



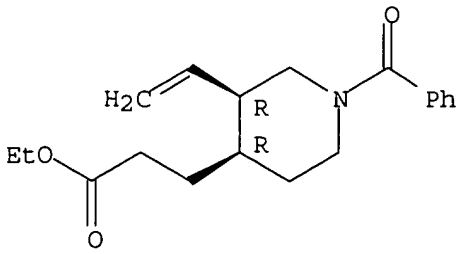
RN 42881-64-1 CAPLUS
CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, (3S-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



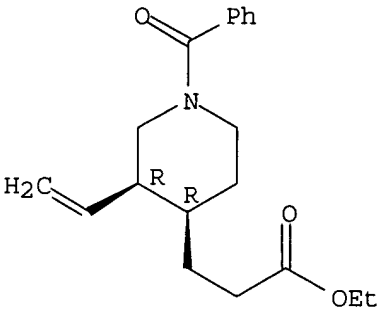
L3 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:466634 CAPLUS
DOCUMENT NUMBER: 79:66634
TITLE: Reinvestigation of the classical synthesis of Cinchona alkaloids. I. New synthesis of homomeroquinene and quinotoxine
AUTHOR(S): Grethe, Guenter; Lee, Hsi Lin; Mitt, Toomas; Uskokovic, Milan R.
CORPORATE SOURCE: Chem. Res. Dep., Hoffmann-La Roche Inc., Nutley, NJ, USA
SOURCE: Helvetica Chimica Acta (1973), 56(5), 1485-94
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 79:66634
GI For diagram(s), see printed CA Issue.
AB N-Benzoylhomomeroquinene ethyl ester (I) was prepared from cis-3-ethyl-4-piperidinepropionic acid Et ester in 6 steps and then converted to quinotoxine (II) by reaction with 4-lithio-6-methoxyquinoline followed by basic hydrolysis.
IT 26847-64-3P 26847-66-5P 42881-64-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 26847-64-3 CAPLUS
CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



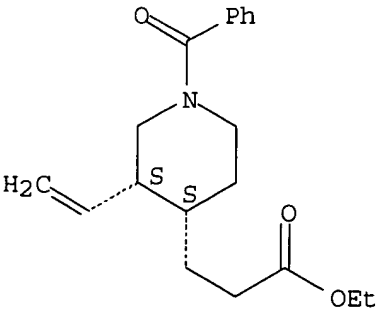
RN 26847-66-5 CAPLUS
CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, (3R-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 42881-64-1 CAPLUS
CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, (3S-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:448685 CAPLUS
DOCUMENT NUMBER: 77:48685
TITLE: Synthesis of 9-epi-quinine and 9-epi-quinidine
AUTHOR(S): Grethe, G.; Gutzwiller, J.; Lee, H. L.; Uskokovic, M. R.
CORPORATE SOURCE: Chem. Res. Dep., Hoffmann-La Roche Inc., Nutley, NJ, USA
SOURCE: Helvetica Chimica Acta (1972), 55(3), 1044-7
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.

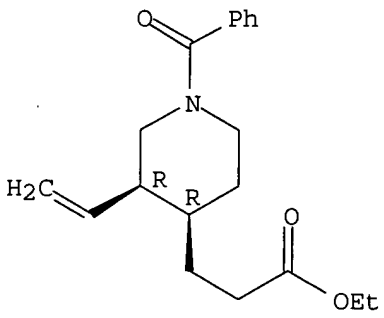
AB A mixture of 9-epiquinine (I) and 9-epiquinidine (II) is prepared from N-benzoyl-hormomeroquinene (III) in a series of reactions in a stereoselective synthesis. III is converted to the Et ester which is treated with 6-methoxy-4-quinolyllithium to give N-benzoylquinotozine (IV), IV is chlorinated by (Me2CH)2NCl to give epimeric α-chloro ketones which are converted to a pair of threo chlorohydrins. The chlorohydrins are treated with KOH at 20° and debenzoylated to give epoxides, and the epoxides are heated in PhMe containing MeOH to 2:1 mixture of I and II.

IT 26847-66-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 26847-66-5 CAPLUS

CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, (3R-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:90696 CAPLUS
DOCUMENT NUMBER: 72:90696
TITLE: Antimalarial dihydroquinines, dihydroquinidines, dihydrocinchonines, and dihydrocinchonidines
INVENTOR(S): Gutzwiller, Juerg A. W.; Uskokovic, Milan R.
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co., A.-G.
SOURCE: Ger. Offen., 96 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1933599	A	19700226	DE 1969-1933599	19690702
CH 521975	A	19720430	CH 1969-521975	19690626
CH 533123	A	19730315	CH 1971-14029	19690626
BE 735450	A	19700102	BE 1969-735450	19690701
FR 2012151	A5	19700313	FR 1969-22135	19690701
AT 319481	B	19741227	AT 1969-6269	19690701
NL 6910144	A	19700106	NL 1969-10144	19690702
NL 166475	B	19810316		
NL 166475	C	19810817		
GB 1253741	A	19711117	GB 1969-1253741	19690702
CA 956312	A1	19741015	CA 1969-55885	19690702
SE 375775	B	19750428	SE 1972-6590	19690702
IL 32534	A1	19750728	IL 1969-32534	19690702
DK 136069	B	19770808	DK 1969-3591	19690702
DE 1967178	C2	19841122	DE 1969-1967178	19690702

AT 7100491	A	19770515	AT 1971-491		19710121
AT 341115	B	19780125			
JP 49015278	B4	19740413	JP 1971-39235		19710604
CA 962682	A2	19750211	CA 1971-126551		19711101
US 3753992	A	19730821	US 1971-212648		19711227
US 3857846	A	19741231	US 1973-354822		19730426
US 3869461	A	19750304	US 1973-354838		19730426
PRIORITY APPLN. INFO.:			US 1968-741913	A	19680702
			US 1969-837304	A2	19690627
			AT 1969-6269	A	19690701
			CA 1969-55885	A3	19690702
			US 1971-104785	A2	19710107
			US 1971-212648	A3	19711227

GI For diagram(s), see printed CA Issue.

AB The title antiarrhythmic and antimalarial compds. (I), (II), (III), and (IV), their racemates, optical antipodes and salts, as well as their starting materials were prepared Thus, 1.5 g V (R = OMe, R1 = R2 = H) in 120 ml CH_2Cl_2 was heated 16 hr at 20° under N with 2.5 ml 17% NaOCl to give 1.65 g crude V (R = OMe, R1 = H, R2 = Cl), which on treatment in 10 ml CH_2Cl_2 with 80 ml H_3PO_4 for 4 hr at 20° gave 930 mg I [R = H, (R1R2 =) O] (Ia), m. 102-4°, [α]25D 71° (c 1.1, EtOH).

Similarly prepared were dl-II [R = H, (R1R2 =) O] (IIa), m. 100-4°; 1:1 mixture of Ia and IIa, m. 80-3°; quinidinone, m. 98-101°, [α]25D 72.6° (c 0.99, EtOH); 1:1 mixture of III [R = H, R1 = OMe, (R2R3 =) O] and IV [R = H, R1 = OMe, (R2R3 =) O](IVa), m. 103-8°, [α]25D 16° (c 0.27, EtOH); dl-IVa, m. 115-18°; 1:1 mixture of III [R = R1 = OMe, (R2R3 =) O] (IIIa) and IV [R = R1 = OMe, (R2R3 =) O] (IVb); mixture of dl-IIIa and dl-IVb; mixture of III [R = Cl, R1 = H, (R2R3 =) O] and IV [R = Cl, R1 = H, (R2R3 =) O], m. 97.5-100.5°; 1:1 mixture of III [R = Me, R1 = H, (R2R3 =) O] (IIIb) and IV [R = Me, R1 = H, (R2R3 =) O], m. 105-8°. Dropwise addition of 25.4 g VIg in 250 ml tetrahydrofuran to 26.9 g tert-BuOK and 25.8 g 7-methoxy-4-ethoxycarbonylquinoline in 400 ml tetrahydrofuran within 30 min under N and refluxing gave Et cis-α-(1-benzoyl-3-ethyl-4-piperidylmethyl)-β-oxo-β-(7-methoxy-4-quinolyl)propionate, which on refluxing 21 hr with HCl gave dl-V (R = R2= H, R1 = OMe) (dl-Va), dibenzoyl-d-tartrate m. 174-5.5°. Similarly prepared were (-)-Va, dibenzoyl-d-tartrate, m.177-9°, [α]26D -39.6° (c 0.5, 1:2 EtOH-$CHCl_3$); V (R = R1 = OMe), R2 =H [(-)-Vb], dibenzoyl-d-tartrate, m. 161.5-3.5°, [α]25D -37.7° (c1.02, 1:2 EtOH-$CHCl_3$); dl-Vb; dl-(V) (R = Cl, R1 = R2 = H); dl-V (R = Me, R1 = R2 = H). Stereoselective reduction of 2 g Ia in 150 ml MePh with 4.8 ml 25% $(iso\text{-}Bu)_2AlH$ in MePh at 20° under N gave 1.9 g I (R = R1 = H,R2 = OH) (Ib), m. 168-9°, [α]22D 227.9° (c 0.896, EtOH). Similarly prepared were a 1:1 mixture of Ib and II (R = R1 = H, R2 = OH) (IIb), [α]24.5D 62.2° (c 1.64, EtOH); dl-IIb, m. 172-4Z; dl-Ib, m. 152-4.5°; quinidine, m. 169-71°, [α]25D 264.3° (c 0.98, EtOH); α(S)-[5-(R)-vinyl-4(S)-quinuclidin-2(R)-yl]-7-chloro-4-quinolinemethanol, m. 247-50°, [α]25D 196° (c 0.88; 4:1 EtOH-CH_2Cl_2); its α(R),2(S) isomer, m. 165-9°, [α]25D -67° (c 0.90, EtOH); III (R = R2 = H, R1 = OMe, R3 = OH) (IIIc), m. 231-3°, [α]25D 169.5° (c 1, EtOH); IV (R = R2 = H, R1 = OMe, R3 = OH) (IVd), m. 162.5°, [α]25D -80.3° (c 0.98, EtOH); dl-IVd, m. 155-7°; dl-IIIc, m. 217-19°; III (R = R1= OMe, R2 = H, R3 = OH) (IIId), m. 116-18°, [α]25D 182.2°(c 0.95, EtOH); IV (R = R1 = OMe, R2 = H, R3 = OH) (IVe), [α]25D -87.3 (c 0.68, EtOH); dl-IIId.2HCl, m. 221-5° (decomposition); dl-IVe, m. 155-7°, dihydrochloride m. 208-10° (decomposition); dl-III (R = Cl, R1 = R2 = H, R3 = OH), m. 172.5-3.5°, dihydrochloride m. 218-21° (decomposition); dl-IV (R = Cl, R1 = R2 = H, R3 = OH), m. 100-2°, dihydrochloride m. 219-20° (decomposition); dl-III (R = Me, R1 = R2 = H, R3 = OH) (IIIe), m. 153.5-5.0°, dihydrochloride, m. 219-20°

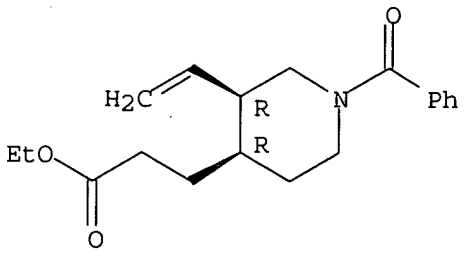
(decomposition); dl-IV (R = Me, R1 = R2 = H, R3 = OH) (IVf), m. 216-18°, dihydrochloride m. 213-16° (decomposition). Reduction of 0.308 g of a mixture of IIIb and IVc in 20 ml MeOH with NaBH4 60 min at 0° gave 0.157 g of a mixture of dl-epi-IIIe and dl-epi-IVf as well as 0.02 g dl-IIIe and 0.023 g dl-IVf. III (R = R2 = H, R1 = Cl, R3 = OH) (0.743 g), m. 278-9°, [α]20D 159.7° (c 0.73; 9:1 EtOH-HOAc), was prepared by treatment of 1.06 g 7'-chlorocinchonine-2HCl-H2O in 500 ml MeOH with 2.5 ml 99% H2NNH2.H2O and .apprx.10 mg CuSO4 for 2 days at room temperature

A solution of 5.253 g dl-II (R = R1 = H, R2 = OH) (IIb) in 20ml MeOH and 16.1 ml N H2SO4 was cooled to 0° to give IIb.H2SO4.0.5H2O, m. 210-13°. Similar treatment of dl-I (R = R1 = H, R2 = OH) (Ib) gave Ib.H2SO4.0.75H2O, m. 208-11°. dl-cis-VIa was prepared (a) by chlorination of 1.064 g dl-cis-VIb in 30 ml Et2O with 30 ml 16.9% NaOCl at room temperature in 0.9 g yield,or (b) by chlorination of 15 g dl-cis-VIb in 100 ml Et2O with 11 g N-chlorosuccinimide in 200 ml Et2O under N 1 hr at room temperature in18 g yield. VIa (18 g) in 150 ml trifluoroacetic acid was rearranged by 5-hr irradiation at 10° to give dl-cis-VIc. VIc (40 g) on reaction with 26 g BzCl in 400 ml C6H6 and K2CO3 2 hr gave 22.3 g dl-cis-VId. dl-cis-VIe was prepared (a) by refluxing 44 hr 3.5 g VId and 2.3 g NaI in 120 ml MeCOEt and treatment of 4 g of the obtained VIf with 2.5 g AgF in 120 ml pyridine in 1.605 g yield, or (b) by heating 5 hr, 0.5 g VId with glass powder at 190°/0.025 mm in 99 mg yield. Similarly prepared were 3(S),4(S)-VIe and its 3(R),4(R) isomer.

IT 26847-64-3P 26847-65-4P 26847-66-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

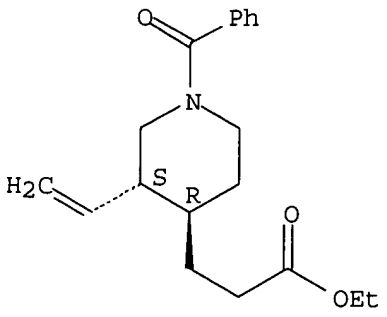
RN 26847-64-3 CAPLUS
CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 26847-65-4 CAPLUS
CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 26847-66-5 CAPLUS
CN 4-Piperidinepropanoic acid, 1-benzoyl-3-ethenyl-, ethyl ester, (3R-cis)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.